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PHY1520H Graduate Quantum Mechanics. Lecture 20: Perturbation theory. Taught by Prof. Arun Paramekanti

Disclaimer Peeter's lecture notes from class. These may be incoherent and rough.

These are notes for the UofT course PHY1520, Graduate Quantum Mechanics, taught by Prof. Paramekanti, covering ch. 5 [1] content.

1.1 Simplest perturbation example.

Given a 2×2 Hamiltonian $H = H_0 + V$, where

$$H = \begin{bmatrix} a & c \\ c^* & b \end{bmatrix}, \tag{1.1}$$

note that if $c = 0$ is

$$H = H_0 = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}. \tag{1.2}$$

The off diagonal terms can be considered to be a perturbation

$$V = \begin{bmatrix} 0 & c \\ c^* & 0 \end{bmatrix}, \tag{1.3}$$

with $H = H_0 + V$.

Energy levels after perturbation We can solve for the eigenvalues of H easily, finding

$$\lambda_\pm = \frac{a+b}{2} \pm \sqrt{\left(\frac{a-b}{2}\right)^2 + \left|c\right|^2}. \tag{1.4}$$

Plots of a few a, b variations of $\lambda_\pm$ are shown in fig. 1.1. The quadratic (non-degenerate) domain is found near the $c = 0$ points of all but the first ($a = b$) plot, and the degenerate (linear in $\left|c\right|^2$) regions are visible for larger values of c.

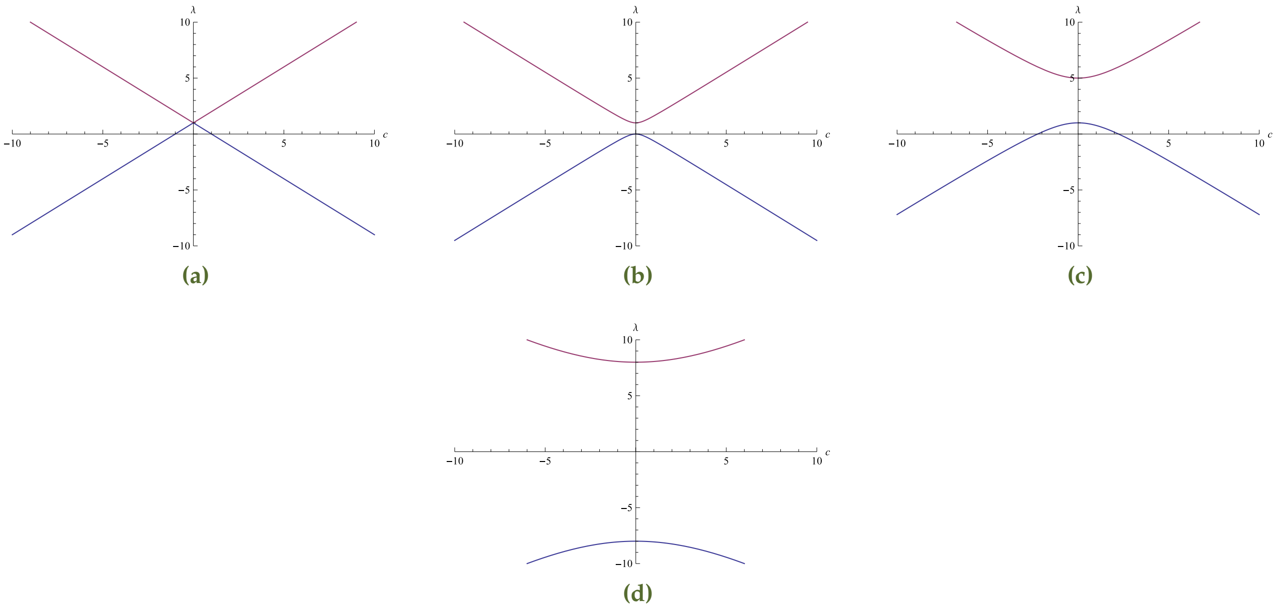

Figure 1.1: Plots of $\lambda_\pm$ for $(a, b) \in \{(1, 1), (1, 0), (1, 5), (-8, 8)\}$

Some approximations Suppose that $|c| \ll |a - b|$, then

$$\lambda_\pm \approx \frac{a+b}{2} \pm \left|\frac{a-b}{2}\right| \left(1 + 2\frac{|c|^2}{|a-b|^2}\right). \tag{1.5}$$

If $a > b$, then

$$\lambda_\pm \approx \frac{a+b}{2} \pm \frac{a-b}{2} \left(1 + 2\frac{|c|^2}{(a-b)^2}\right). \tag{1.6}$$

$$\begin{aligned}
\lambda_+ &= \frac{a+b}{2} + \frac{a-b}{2} \left(1 + 2\frac{|c|^2}{(a-b)^2}\right) \\
&= a + (a-b)\frac{|c|^2}{(a-b)^2} \\
&= a + \frac{|c|^2}{a-b},
\end{aligned} \tag{1.7}$$

and

$$\begin{aligned}\lambda_- &= \frac{a+b}{2} - \frac{a-b}{2}\left(1 + 2\frac{|c|^2}{(a-b)^2}\right) \\ &= b + (a-b)\,\frac{|c|^2}{(a-b)^2} \\ &= b + \frac{|c|^2}{a-b}.\end{aligned} \tag{1.8}$$

This adiabatic evolution displays a "level repulsion", quadratic in $|c|$, and is described as a non-degenerate permutation.

If $|c| \gg |a-b|$, then

$$\begin{aligned}\lambda_\pm &= \frac{a+b}{2} \pm |c|\sqrt{1 + \frac{1}{|c|^2}\left(\frac{a-b}{2}\right)^2} \\ &\approx \frac{a+b}{2} \pm |c|\left(1 + \frac{1}{2|c|^2}\left(\frac{a-b}{2}\right)^2\right) \\ &= \frac{a+b}{2} \pm |c| \pm \frac{(a-b)^2}{8|c|}.\end{aligned} \tag{1.9}$$

Here we loose the adiabaticity, and have "level repulsion" that is linear in $|c|$. We no longer have the sign of $a-b$ in the expansion. This is described as a degenerate permutation.

1.2 General non-degenerate perturbation

Given an unperturbed system with solutions of the form

$$H_0 \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(0)}\right\rangle, \tag{1.10}$$

we want to solve the perturbed Hamiltonian equation

$$(H_0 + \lambda V)\left|n\right\rangle = \left(E_n^{(0)} + \Delta n\right)\left|n\right\rangle. \tag{1.11}$$

Here Δn is an energy shift as that goes to zero as $\lambda \to 0$. We can write this as

$$\left(E_n^{(0)} - H_0\right)\left|n\right\rangle = (\lambda V - \Delta_n)\left|n\right\rangle. \tag{1.12}$$

We are hoping to iterate with application of the inverse to an initial estimate of $\left|n\right\rangle$

$$\left|n\right\rangle = \left(E_n^{(0)} - H_0\right)^{-1}(\lambda V - \Delta_n)\left|n\right\rangle. \tag{1.13}$$

This gets us into trouble if $\lambda \to 0$, which can be fixed by using

$$\left|n\right\rangle = \left(E_n^{(0)} - H_0\right)^{-1}(\lambda V - \Delta_n)\left|n\right\rangle + \left|n^{(0)}\right\rangle, \tag{1.14}$$

which can be seen to be a solution to eq. (1.12). We want to ask if

$$(\lambda V - \Delta_n) |n\rangle , \tag{1.15}$$

contains a bit of $\left|n^{(0)}\right\rangle$? To determine this act with $\left\langle n^{(0)}\right|$ on the left

$$\begin{aligned}\left\langle n^{(0)}\right| (\lambda V - \Delta_n) |n\rangle &= \left\langle n^{(0)}\right| \left(E_n^{(0)} - H_0\right) |n\rangle \\ &= \left(E_n^{(0)} - E_n^{(0)}\right) \left\langle n^{(0)} \middle| n\right\rangle \\ &= 0.\end{aligned} \tag{1.16}$$

This shows that $|n\rangle$ is entirely orthogonal to $\left|n^{(0)}\right\rangle$.
Define a projection operator

$$P_n = \left|n^{(0)}\right\rangle \left\langle n^{(0)}\right| , \tag{1.17}$$

which has the idempotent property $P_n^2 = P_n$ that we expect of a projection operator.
Define a rejection operator

$$\begin{aligned}\overline{P}_n &= 1 - \left|n^{(0)}\right\rangle \left\langle n^{(0)}\right| \\ &= \sum_{m\neq n} \left|m^{(0)}\right\rangle \left\langle m^{(0)}\right| .\end{aligned} \tag{1.18}$$

Because $|n\rangle$ has no component in the direction $\left|n^{(0)}\right\rangle$, the rejection operator can be inserted much like we normally do with the identity operator, yielding

$$|n\rangle ' = \left(E_n^{(0)} - H_0\right)^{-1} \overline{P}_n (\lambda V - \Delta_n) |n\rangle + \left|n^{(0)}\right\rangle , \tag{1.19}$$

valid for any initial $|n\rangle$.

Power series perturbation expansion Instead of iterating, suppose that the unknown state and unknown energy difference operator can be expanded in a λ power series, say

$$|n\rangle = |n_0\rangle + \lambda |n_1\rangle + \lambda^2 |n_2\rangle + \lambda^3 |n_3\rangle + \cdots \tag{1.20}$$

and

$$\Delta_n = \Delta_{n_0} + \lambda\Delta_{n_1} + \lambda^2\Delta_{n_2} + \lambda^3\Delta_{n_3} + \cdots \tag{1.21}$$

We usually interpret functions of operators in terms of power series expansions. In the case of $\left(E_n^{(0)} - H_0\right)^{-1}$, we have a concrete interpretation when acting on one of the unperturbed eigenstates

$$\frac{1}{E_n^{(0)} - H_0} \left|m^{(0)}\right\rangle = \frac{1}{E_n^{(0)} - E_m^0} \left|m^{(0)}\right\rangle . \tag{1.22}$$

This gives

$$|n\rangle = \frac{1}{E_n^{(0)} - H_0} \sum_{m \neq n} \left|m^{(0)}\right\rangle \left\langle m^{(0)}\right| (\lambda V - \Delta_n) |n\rangle + \left|n^{(0)}\right\rangle , \tag{1.23}$$

or

$$\boxed{|n\rangle = \left|n^{(0)}\right\rangle + \sum_{m \neq n} \frac{\left|m^{(0)}\right\rangle \left\langle m^{(0)}\right|}{E_n^{(0)} - E_m^{(0)}} (\lambda V - \Delta_n) |n\rangle .} \tag{1.24}$$

From eq. (1.12), note that

$$\Delta_n = \frac{\left\langle n^{(0)}\right| \lambda V |n\rangle}{\langle n^0 | n\rangle}, \tag{1.25}$$

however, we will normalize by setting $\langle n^0 | n\rangle = 1$, so

$$\boxed{\Delta_n = \left\langle n^{(0)}\right| \lambda V |n\rangle .} \tag{1.26}$$

to $O(\lambda^0)$ If all $\lambda^n, n > 0$ are zero, then we have

$$|n_0\rangle = \left|n^{(0)}\right\rangle + \sum_{m \neq n} \frac{\left|m^{(0)}\right\rangle \left\langle m^{(0)}\right|}{E_n^{(0)} - E_m^{(0)}} \left(-\Delta_{n_0}\right) |n_0\rangle \tag{1.27a}$$

$$\Delta_{n_0} \left\langle n^{(0)} \middle| n_0 \right\rangle = 0 \tag{1.27b}$$

so

$$\begin{aligned} |n_0\rangle &= \left|n^{(0)}\right\rangle \\ \Delta_{n_0} &= 0. \end{aligned} \tag{1.28}$$

to $O(\lambda^1)$ Requiring identity for all λ^1 terms means

$$|n_1\rangle \lambda = \sum_{m \neq n} \frac{\left|m^{(0)}\right\rangle \left\langle m^{(0)}\right|}{E_n^{(0)} - E_m^{(0)}} \left(\lambda V - \Delta_{n_1} \lambda\right) |n_0\rangle , \tag{1.29}$$

so

$$|n_1\rangle = \sum_{m \neq n} \frac{\left|m^{(0)}\right\rangle \left\langle m^{(0)}\right|}{E_n^{(0)} - E_m^{(0)}} \left(V - \Delta_{n_1}\right) |n_0\rangle . \tag{1.30}$$

With the assumption that $\left|n^{(0)}\right\rangle$ is normalized, and with the shorthand

$$V_{mn} = \left\langle m^{(0)}\right| V \left|n^{(0)}\right\rangle , \tag{1.31}$$

that is

$$
\begin{aligned}
|n_1\rangle &= \sum_{m\neq n} \frac{|m^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} V_{mn} \\
\Delta_{n_1} &= \left\langle n^{(0)} \right| V \left| n^0 \right\rangle = V_{nn}.
\end{aligned}
\tag{1.32}
$$

to $O(\lambda^2)$ The second order perturbation states are found by selecting only the λ^2 contributions to

$$
\lambda^2 |n_2\rangle = \sum_{m\neq n} \frac{|m^{(0)}\rangle \langle m^{(0)}|}{E_n^{(0)} - E_m^{(0)}} \left(\lambda V - (\lambda \Delta_{n_1} + \lambda^2 \Delta_{n_2})\right) \left(|n_0\rangle + \lambda |n_1\rangle\right). \tag{1.33}
$$

Because $|n_0\rangle = |n^{(0)}\rangle$, the $\lambda^2 \Delta_{n_2}$ is killed, leaving

$$
\begin{aligned}
|n_2\rangle &= \sum_{m\neq n} \frac{|m^{(0)}\rangle \langle m^{(0)}|}{E_n^{(0)} - E_m^{(0)}} \left(V - \Delta_{n_1}\right) |n_1\rangle \\
&= \sum_{m\neq n} \frac{|m^{(0)}\rangle \langle m^{(0)}|}{E_n^{(0)} - E_m^{(0)}} \left(V - \Delta_{n_1}\right) \sum_{l\neq n} \frac{|l^{(0)}\rangle}{E_n^{(0)} - E_l^{(0)}} V_{ln},
\end{aligned}
\tag{1.34}
$$

which can be written as

$$
|n_2\rangle = \sum_{l,m\neq n} \left| m^{(0)} \right\rangle \frac{V_{ml} V_{ln}}{\left(E_n^{(0)} - E_m^{(0)}\right)\left(E_n^{(0)} - E_l^{(0)}\right)} - \sum_{m\neq n} \left| m^{(0)} \right\rangle \frac{V_{nn} V_{mn}}{\left(E_n^{(0)} - E_m^{(0)}\right)^2}. \tag{1.35}
$$

For the second energy perturbation we have

$$
\lambda^2 \Delta_{n_2} = \left\langle n^{(0)} \right| \lambda V \left(\lambda |n_1\rangle\right), \tag{1.36}
$$

or

$$
\begin{aligned}
\Delta_{n_2} &= \left\langle n^{(0)} \right| V |n_1\rangle \\
&= \left\langle n^{(0)} \right| V \sum_{m\neq n} \frac{|m^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} V_{mn}.
\end{aligned}
\tag{1.37}
$$

That is

$$
\Delta_{n_2} = \sum_{m\neq n} \frac{V_{nm} V_{mn}}{E_n^{(0)} - E_m^{(0)}}. \tag{1.38}
$$

to $O(\lambda^3)$ Similarly, it can be shown that

$$
\Delta_{n_3} = \sum_{l,m\neq n} \frac{V_{nm} V_{ml} V_{ln}}{\left(E_n^{(0)} - E_m^{(0)}\right)\left(E_n^{(0)} - E_l^{(0)}\right)} - \sum_{m\neq n} \frac{V_{nm} V_{nn} V_{mn}}{\left(E_n^{(0)} - E_m^{(0)}\right)^2}. \tag{1.39}
$$

In general, the energy perturbation is given by

$$
\Delta_n^{(l)} = \left\langle n^{(0)} \right| V \left| n^{(l-1)} \right\rangle. \tag{1.40}
$$

Bibliography

[1] Jun John Sakurai and Jim J Napolitano. *Modern quantum mechanics*. Pearson Higher Ed, 2014. 1